ARKIV FÖR FYSIK Band 11 nr 37

Communicated 14 November 1956 by IVAR WALLER and O. H. FAXÉN

On a modified Hulthén potential

By S. G. M. GUSTAVI

Introduction

Meson theory has long ago predicted highly singular potentials of the form $e^{-\mu r}/(\mu r)$, $e^{-\mu r}/(\mu r)^2$ and even $e^{-\mu r}/(\mu r)^3$ for the two-nucleon interaction. Because of analytical difficulties these potentials have been treated almost exclusively with numerical methods, especially when they are used with a "cut off" which removes the singularity, as is usual and in some cases necessary. Being forced to numerical solutions, however, one loses much of the general survey of the problem and therefore it may be of some value to construct modified potentials, similar to those above in form and physical properties, which can be treated analytically. For the Yukawa potential we already have the well-known Hulthén potential $e^{-\mu r}/(1-e^{-\mu r})$ [1], and here we shall discuss a natural modification of this potential to the form $e^{-\mu r}/(1-e^{-\mu r})^2$, which is as easy to handle analytically as the original one and which may be used as an approximation to the meson potential $e^{-\mu r}/(\mu r)^2$. At least the singular properties at the origin must be the same for the approximative and the original potential and for large values of μr where the approximation is not very good both potentials are so small in value as to be neglected. An analogous approximation for the potential $e^{-\mu r}/(\mu r)^3$ is of course also conceivable but in this case it seems as if the approximative potential does not have any special advantage over the original one.

Solution of the wave equation

In the S state which is the only one of interest here the radial wave equation for the deuteron system may be written in common notation

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+\frac{M}{\hbar^2}(E-V(r))\right]R(r)=0, \tag{1}$$

where M is the nucleon mass, E the energy and $V(r)$ the (central) potential. Here

$$V(r)=-V_0\frac{e^{-\mu r}}{(1-e^{-\mu r})^2}, \tag{2}$$

where V_0 is a positive constant. After the usual transformation $R(r)=u(r)/r$ we get from (1):

$$\left[\frac{d^2}{dr^2}+k^2\right]u(r)=\frac{M}{\hbar^2}V(r)\,u(r), \tag{3}$$

where $k^2 = ME/\hbar^2$. In the case of an ordinary Hulthén potential this equation can be transformed into a hypergeometric differential equation by the transformation

$$u = e^{-ikr} F(e^{-\mu r}); \qquad e^{-\mu r} = z$$

(see [1] and [2]), and this is suited also for our problem. After applying it to equation (3) with $V(r)$ taken as the modified Hulthén potential (2) we get

$$\left[\frac{d^2}{dz^2} + \left(1 + \frac{2ik}{\mu}\right)\frac{1}{z}\frac{d}{dz} + \frac{v_0}{z(1-z)^2}\right] F(z) = 0, \tag{4}$$

where $v_0 = (M/\hbar^2)(V_0/\mu^2)$. This is not a hypergeometric equation, but it is, however, a second-order differential equation with three regular singular points and can thus be transformed into a hypergeometric equation [3]. The suitable transformation is

$$F(z) = (1-z)^t f(z), \tag{5}$$

where t is one of the roots of the indical equation for the singular point $z = 1$ ($r = 0$):

$$t(t-1) + v_0 = 0. \tag{6}$$

We shall in the following denote these two roots by

$$t_1 = \tfrac{1}{2} + \sqrt{\tfrac{1}{4} - v_0}, \qquad t_2 = \tfrac{1}{2} - \sqrt{\tfrac{1}{4} - v_0}, \tag{7}$$

while t without index may represent any of them. The transformation (5) will bring (4) into the form

$$z(z-1)f''(z) + \left[\left(1 + 2t + 2\frac{ik}{\mu}\right)z - \left(1 + \frac{2ik}{\mu}\right)\right] f'(z) + \left[t^2 + 2t\frac{ik}{\mu}\right] f(z) = 0. \tag{8}$$

This is a hypergeometric equation, the general form of which may be written [4]:

$$z(z-1)g''(z) + [(1 + a + b)z - c]\, g'(z) + ab\, g(z) = 0. \tag{9}$$

Comparison between (8) and (9) gives

$$a = t; \qquad b = t + \frac{2ik}{\mu}; \qquad c = 1 + \frac{2ik}{\mu}. \tag{10}$$

The solutions of (9) are most suitably given in terms of series solutions about some or other of the three singular points of the equation, and all these series solutions can be expressed with help of the hypergeometric series [4]:

$$\begin{aligned} F(a, b, c; z) &= 1 + \frac{ab}{c} z + \frac{a(a+1)\,b(b+1)}{\underline{|2}\, c(c+1)} z^2 + \cdots \\ &= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_0^\infty \frac{\Gamma(a+n)\Gamma(b+n)}{\underline{|n}\, \Gamma(c+n)} z^n. \end{aligned} \tag{11}$$

We are primarily interested in two kinds of solutions of (3) (and correspondingly of (8)): for the discussion of bound state problems we need the negative energy ($ik = \varkappa$,

$\varkappa$ real and positive) solutions that are regular at infinity and for low energy scattering problems we need the zero energy ($k = 0$) solutions.

We begin with the first case. The general series solution of (9) about $z = 0$ ($r = \infty$) is [4]:

$$g(z) = A\,F(a,b,c;\,z) + B z^{1-c} F(a-c+1, b-c+1, 2-c;\,z),$$

which gives according to (10):

$$f(z) = A\,F\left(t, t+\frac{2\varkappa}{\mu},\ 1+\frac{2\varkappa}{\mu};\,z\right) + B z^{-\frac{2\varkappa}{\mu}} F\left(t-\frac{2\varkappa}{\mu},\ t,\ 1-\frac{2\varkappa}{\mu};\,z\right). \tag{12}$$

From this it is easy to see that the solution of the wave equation (3) for $ik = \varkappa$ ($\varkappa$ real and positive) that is regular at infinity (for $r = \infty$ or $z = 0$) must be of the form

$$u(\varkappa;\,r) = e^{-\varkappa r}(1-e^{-\mu r})^t F\left(t, t+\frac{2\varkappa}{\mu},\ 1+\frac{2\varkappa}{\mu};\ e^{-\mu r}\right). \tag{13}$$

This solution at first sight seems to depend on the choice of t in an essential way but in fact it does not. In order to realize that and to obtain a form of the solution which is sometimes more useful than (14) we employ the analytic continuation formula [4]

$$F(a, b, c;\,z) = \frac{\Gamma(c)\,\Gamma(c-a-b)}{\Gamma(c-a)\,\Gamma(c-b)} F(a, b, a+b-c+1;\ 1-z) +$$
$$+ \frac{\Gamma(c)\,\Gamma(a+b-c)}{\Gamma(a)\,\Gamma(b)} (1-z)^{c-a-b} F(c-a,\ c-b,\ c-a-b+1;\ 1-z), \tag{14}$$

which inside the common region of convergence connects the ordinary hypergeometric series with the series solutions of equation (9) about $z = 1$. (13) and (14) give

$$u(\varkappa;\,r) = \frac{\Gamma\left(1+\frac{2\varkappa}{\mu}\right)}{t_2-t_1} e^{-\varkappa r}\left[\frac{\Gamma(2t_2)}{\Gamma(t_2)\,\Gamma\left(t_2+\frac{2\varkappa}{\mu}\right)}(1-e^{-\mu r})^{t_1} F\left(t_1, t_1+\frac{2\varkappa}{\mu}, 2t_1;\ 1-e^{-\mu r}\right) - \right.$$
$$\left. - \frac{\Gamma(2t_1)}{\Gamma(t_1)\,\Gamma\left(t_1+\frac{2\varkappa}{\mu}\right)}(1-e^{-\mu r})^{t_2} F\left(t_2, t_2+\frac{2\varkappa}{\mu};\ 2t_2;\ 1-e^{-\mu r}\right)\right], \tag{15}$$

where we have taken $t = t_1$ in (13) and used the relations

$$t_1 + t_2 = 1 \quad \text{and} \quad \Gamma(z+1) = z\,\Gamma(z).$$

Apart from a minus sign the choice $t = t_2$ in (13) will obviously give the same result. It may be remarked that (15) shows $u(\varkappa;\,r)$ to be real also in the case of complex t values ($v_0 > \frac{1}{4}$), because t_2 is then the complex conjugate of t_1.

For $\mu r \ll 1$ the hypergeometric series in (15) are approximately constant while $(1-e^{-\mu r})^{t_1} \approx (\mu r)^{t_1}$ and $(1-e^{-\mu r})^{t_2} \approx (\mu r)^{t_2}$. Now from (7) if $v_0 > 0$ we get $0 < Re(t) < 1$.

Consequently $u(\varkappa; r)$ always goes to zero with r, while the original radial function $R(\varkappa; r) = u(\varkappa; r)/r$ is always singular at the origin. If the t values are real, that is if $v_0 \leq \frac{1}{4}$ the general form of the wave function is rather simple; it is always positive and the second derivative changes sign at one place only. In the case of complex t values ($v_0 > \frac{1}{4}$), on the other hand, the wave function oscillates with a frequency which goes to infinity as $r \to 0$, because of factors of the form $\cos(\nu \log \mu r)$, where ν is the imaginary part of t_1 (or t_2). The distinction between real and complex values is a very important one and we shall in the following denote the potential as *undercritical* or *overcritical* if $v_0 \leq \frac{1}{4}$ or $> \frac{1}{4}$ respectively.

We now turn to the zero energy case ($k = 0$). The general series solution of (9) about the singular point $z = 1$ (which corresponds to $r = 0$) is:

$$g(z) = A\,F(a,b,a+b-c+1;\,1-z) + B(1-z)^{c-a-b}\,F(c-b,c-a,c-a-b+1;\,1-z). \tag{16}$$

For $k = 0$ this gives two independent solutions of the equation (3) which may be written

$$\left.\begin{aligned} u_0^{(1)}(r) &= (1-e^{-\mu r})^{t_1}\,F(t_1,\,t_1,\,2\,t_1;\,1-e^{-\mu r}),\\ u_0^{(2)}(r) &= (1-e^{-\mu r})^{t_2}\,F(t_2,\,t_2,\,2\,t_2;\,1-e^{-\mu r}).\end{aligned}\right\} \tag{17}$$

For small r values the behaviour of the functions above is quite similar to that of $u(\varkappa; r)$ and especially we can distinguish between an undercritical and an overcritical case in the same way. In the overcritical case the functions (17) are not real, however, and it is then perhaps more natural to take the real and imaginary parts of one of them as independent solutions.

The asymptotic behaviour of the zero energy functions for large r values needs some special attention. Let us define a_n according to

$$F(t,\,t,\,2\,t;\,z) = \frac{\Gamma(2\,t)}{\Gamma^2(t)}\sum_{n=0}^{\infty}\frac{\Gamma^2(t+n)}{\Gamma(2\,t+n)}\,\frac{z^n}{\underline{|n}} = \sum_{n=0}^{\infty} a_n\,z^n.$$

A straightforward estimation with help of the Stirling formula for the gamma function will yield the following formula for the asymptotic behaviour of a_n:

$$a_n = \frac{\Gamma(2\,t)}{\Gamma^2(t)}\left(\frac{1}{n} - \frac{t^2}{n^2} + 0\left(\frac{1}{n^3}\right)\right). \tag{18}$$

Let us denote $(1/n)\,[\Gamma(2\,t)/\Gamma^2(t)]$ by b_n and consider the expression

$$(1-e^{-\mu r})^t\left[1 + \sum_{n=1}^{\infty}(a_n - b_n)\,(1-e^{-\mu r})^n\right] + (1-e^{-\mu r})^t\sum_{n=1}^{\infty} b_n\,(1-e^{-\mu r})^n \tag{19}$$

which is identical with $u_0^{(i)}(r)$ if we choose $t = t_i$ ($i = 1, 2$). Because

$$\sum_{n=1}^{\infty}\frac{1}{n}(1-e^{-\mu r})^n = -\log\,[1-(1-e^{-\mu r})] = \mu\,r$$

we have
$$\lim_{r\to\infty}\left[\frac{\Gamma(2\,t)}{\Gamma^2(t)}\,\mu\,r - (1-e^{-\mu r})^t\sum_{n=1}^{\infty} b_n\,(1-e^{-\mu r})^n\right] = 0. \tag{20}$$

The first term in (19), on the other hand, tends to a constant as $r \to \infty$, because, according to (18),

$$c_n = b_n - a_n = \frac{\Gamma(2t)}{\Gamma^2(t)} \left(\frac{t^2}{n^2} + 0 \left(\frac{1}{n^3} \right) \right), \quad (n \geq 1) \tag{21}$$

so that $\sum c_n$ is convergent and we may use Abel's theorem for power series [5] so as to obtain

$$\lim_{r \to \infty} \left[(1 - e^{-\mu r})^t \left(1 + \sum_{n=1}^{\infty} (a_n - b_n)(1 - e^{-\mu r})^n \right) \right]$$

$$= C(t) = 1 - \sum_{n=1}^{\infty} c_n = \frac{\Gamma(2t)}{\Gamma^2(t)} \sum_{0}^{\infty} \left(\frac{\Gamma^2(t+n)}{\Gamma(2t+n)} \frac{1}{\underline{|n}} - \frac{1}{n+1} \right), \tag{22}$$

where by $C(t)$ we have indicated that the constant depends on t. It is easily seen that $C(1) = 0$ and $\lim_{t \to 0} C(t) = 1$, while between these values $C(t)$ is a monotonously decreasing function of t, which must be evaluated numerically by summing the series (22). Putting together the formulae (19), (20) and (22) we get at last the asymptotic expression

$$U_0^{(i)}(r) \underset{r \to \infty}{\sim} C(t_i) + \frac{\Gamma(2\,t_i)}{\Gamma^2(t_i)} \mu r. \tag{23}$$

Before we leave this discussion of the solutions of the differential equation (3) we should perhaps point out that in the case $t_1 = t_2 = \frac{1}{2}$ some of the formulae above must be modified. In this case the two series about $z = 1$ $(r = 0)$ which are represented in (15) and (17) are identical and a second independent solution must be found in the form of a series which contains a logarithmic term and gives a wave function $u(r)$ with a behaviour of the form $\sqrt{r} \log r$ at the origin. Consequently the formula (15) is not valid for $t_1 = t_2 = \frac{1}{2}$ and one of the functions (17) must be replaced by the abovementioned other series.

Physical consequences

The singularity of the modified Hulthén potential at the origin is in some respect a limiting case of what may be allowed. As we have seen all solutions of the radial wave equation (3) goes to zero at the origin either as r^{t_1} or r^{t_2} (or $\sqrt{r} \log r$ for the special case $t_1 = t_2 = \frac{1}{2}$) while the radial function $R(r) = u(r)/r$ is always singular at the origin. This last fact is not a reason for us to reject the potential (in the Dirac theory of the hydrogen atom we have a similar case), but on the other hand it is certainly not possible to accept both r^{t_1} and r^{t_2} as allowed forms of the wave function for small r, because that would destroy the uniqueness of the wave function for positive energies and give us a continuous spectrum for negative energies. As has sometimes been observed in the literature (see for instance [6], where scattering by an inverse cube law force is briefly discussed) the only way of using the potential in physical problems is to accept one of the t values and reject the other one. But this would perhaps not be more than a mathematical device if we could not find any physical support for the procedure.

Now, in the overcritical case $(v_0 > \frac{1}{4})$ it is certainly impossible to make any physical distinction between the two exponential values and thus we must conclude that an overcritical modified Hulthén potential can be used with cut off only. We may, however, treat the undercritical case independently of the overcritical one, although this is perhaps an ambiguous point. When the exponentials are real the "degree of singularity" in the wave function $R(r)$ is not the same for both values and it may seem natural to accept the largest of them (corresponding to t_1) and reject the other one. From a physical standpoint this choice is also supported for instance by a criterion used earlier in the relativistic treatment of the hydrogen atom referred to above (see for instance [7]) and which states that if a potential gives rise to a singularity in the wave function, this singularity must vanish together with the potential if it is to be accepted; this is only the case for the exponential $t = t_1$, which tends to 1 as v_0 approaches zero.

To summarize the situation, we may state that complex exponentials and the exponential t_2 in the real case are unpermissible for physical reasons, while the real exponential t_1 perhaps may be accepted; in any case it is natural to examine the consequences of an acceptance.

Let us first discuss the possibility of bound states for an undercritical potential. If the singularity arising from $(1 - e^{-\mu r})^{t_2}$ is not allowed, the factor $\Gamma(2t_1)/\Gamma(t_1)\Gamma(t_1 + 2\varkappa/\mu)$ in the solution (15) must vanish for a bound state. But in the undercritical case all arguments in these gamma functions are real and positive, thus also the functions themselves (for $t_1 = t_2 = \frac{1}{2}$ we get instead a non-vanishing part of the function, which behaves as $\sqrt{r}\log r$ at the origin). Consequently there are no bound states and, as it ought to be, this conclusion is still valid if we introduce a cut off in the potential, because the wave function $u(\varkappa; r)$ is always positive outside the origin if $v_0 < \frac{1}{4}$. The nonexistence of a bound state for an undercritical potential is also consistent with the fact that the scattering length is negative in this case as is evident from the asymptotic form (23) of the zero energy wave function.

We then turn to the low energy scattering problem. The allowed zero energy solution is (17) with $t = t_1$ and the asymptotic form of this, normalized as in the effective range theory is obtained from (23):

$$1 + \frac{k(t_1)}{C(t_1)}\mu r \quad \text{or} \quad 1 + \frac{k(t_1)}{C(t_1)}\cdot\frac{r}{r_s}, \tag{24}$$

where r_s is the range of the potential and $k(t)$ a notation for $\Gamma(2t)/\Gamma^2(t)$. If we want to adjust the undercritical potential to known singlet scattering data, (24) is to be compared with the form $1 - r/a_s$, where we may take the experimentally given scattering length $a_s = -23.69 \times 10^{-13}$ cm [8]. For a fixed value of t_1, this will give us an expression for r_s:

$$r_s = -a_s\frac{k(t_1)}{C(t_1)}, \tag{25}$$

and it is easy to see that this is a monotonously increasing function of t_1. Now the smallest possible value of t_1 is $\frac{1}{2}$ and the corresponding value of r_s, computed from (25), is $r_s = 8.51 \times 10^{-13}$ cm. But already a very rough estimation shows that this value is much too large to give an effective range of the correct order of size ($r_{os} = 2.4 \pm 0.5 \times 10^{-13}$ cm according to [8]).

If we introduce a cut off on the other hand, it is not difficult to show that in the undercritical case the potential is still too weak to be adjusted even to the singlet scattering data, and in fact it is weaker than the corresponding potential without cut off as it ought to be.

The somewhat disappointing result of our investigation of the undercritical modified Hulthén potential is consequently that this potential alone is too weak to be of any interest for the two-nucleon problem, and this result is certainly also valid for the original meson potential $e^{-\mu r}/(\mu r)^2$. The investigation has shown, however, that the choice of t_1 as the only allowed exponential, gives physical results that are quite analogous to those for a more regular potential.

An overcritical potential, which as we have seen, must be used with cut off, is of cause possible to apply both to the triplet and the singlet case, but unfortunately the wave functions are much more difficult to handle analytically if a cut off is introduced and we shall not here discuss this point any further.

There still remains the possibility, however, to combine an ordinary and an (undercritical) modified Hulthén potential, that is to use a potential of the form

$$V(r) = -V_1 \frac{e^{-\mu r}}{(1-e^{-\mu r})} - V_2 \frac{e^{-\mu r}}{(1-e^{-\mu r})^2},$$

where V_1 and V_2 are constants. In this case also, the wave equation is soluble in terms of hypergeometric functions and the singular properties at the origin are quite the same as for the modified potential alone. Up till now, no detailed calculations have been carried out on the basis of this combined potential, however.

ACKNOWLEDGEMENTS

I want to express my sincere gratitude to the head of the Department, Professor Lamek Hulthén, for his kind interest in this work, and to Professor Masao Sugawara, who has given valuable suggestions and with whom I have discussed parts of the manuscript. Further I am indebted to Tekn. Lic. Bengt Nagel, who has looked through the manuscript.

The work has been carried out under a scholarship from the State Council of Technical Research.

Department of Mathematical Physics, Royal Institute of Technology, Stockholm, October, 1956.

REFERENCES

1. L. Hulthén, Ark. f. Mat., Astr. o. Fysik, Bd *28 A*, N:o 5 (1942).
2. R. Jost, Helv. Phys. Acta *20*, 25 (1947).
3. W. Magnus and F. Oberhettinger, Formeln und Sätze für die speziellen Funktionen der math. Physik, 2. Aufl., Chap. II, § 3. Springer (1948).
4. W. Magnus and F. Oberhettinger, Loc, cit. Chap. II, §§ 1, 2.
5. E. C. Titchmarsh, The Theory of Functions, 2nd Ed., pp. 9 and 229. Oxford Univ. Press (1939).
6. N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions, 2nd. Ed., p. 40. Oxford Univ. Press (1949).
7. A. Sommerfeld, Wellenmechanik, p. 287. Frederich Ungar Publishing Co., New York.
8. L. Hulthén and M. Sugawara, The Two-Nucleon Problem, *in* Handbuch der Physik, vol. 39, Springer (to be published).

Tryckt den 7 februari 1957

Uppsala 1957. Almqvist & Wiksells Boktryckeri AB